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AFM Morphology Study of Si_{1-Y} Ge_Y:H Films Deposited by LF PE CVD from Silane-Germane with Different Dilution

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ABSTRACT

The morphology of Si_{1-Y} Ge_Y:H films in the range of Y=0.23 to 0.9 has been studied by AFM. The films were deposited by Low Frequency (LF) PE CVD at substrate temperature T_s=300 C and discharge frequency f=110 kHz from silane+germane mixture with and without, Ar and H_2 dilution. The films were deposited on silicon and glass substrates. AFM images were taken and analyzed for 2x2 μm^2 area. All the images demonstrated "grain" like structure, which was characterized by the height distribution function F(H) average roughness <H>, standard height deviation R_q, lateral correlation length L_c area distribution function F(s), mean grain area <s>, diameter distribution function F(d), and mean grain diameter <d>. The roughness <H> of the films monotonically increases with Y for all dilutions, but more significantly in the films deposited without dilution. L_c continuously grows with Y in the films deposited without dilution, while more complex behavior L_c(Y) is observed in the films deposited with H- or Ar dilution. The sharpness of F(H) characterized by curtosis γ depends on dilution and the sharpest F(H) are for the films deposited with Ar (γ=5.30,Y=0.23) and without dilution (γ=4.3, Y=0.45). Isothermal annealing caused increase of <H>, L_c in the films deposited with H- and Ar dilutions, while in the films prepared without dilution the behavior was more complex, depending on the substrates. Significant narrowing of the height distribution was observed in the films deposited with H dilution or without dilution

INTRODUCTION

Plasma deposited films have a broad range of applications due to the versatile character of the materials and their compatibility to standard silicon technology. Among them silicon-germanium alloy, $Si_{1-Y}Ge_Y$:H, is a promising material with optical gap less than amorphous silicon films. As a low-bandgap material it can be used in multi-junction solar cells [1,2] photo-detectors [3,4], and un-cooled micro-bolometers [5-7] Despite implementation in devices, $Si_{1-Y}Ge_Y$:H films have been significantly less studied than plasma deposited silicon films. Reviews of earlier works can be found in ref. [8,9]. $Si_{1-Y}Ge_Y$:H films deposited in low frequency (LF) plasma were reported in ref. [10] and more systematically in ref. [11]. In the latter a significant effect of feed gas dilution on electronic properties has been observed. Study of surface morphology, i.e. roughness is an important part of structural characterization. Surface roughness of low temperature PECVD a-Si:H films have been studied by Dalakos et al. [12], who studied roughness evolution during growth. Evolution of roughness in a-SiN_X: films has been reported by Van der Oever et.al.[13]. Nano-crystalline Ge films have been recently studied by Jordan et al. [14, 15]. Grain like structures in AFM images were observed also in solar cells fabricated by RF PECVD [16]. Our previous study has revealed nano-sized grain like structure in AFM images of Si-Ge films deposited by LF PECVD [11, 17].

This study concerns the effect of the dilution of feed gases and annealing on surface morphology with an emphasis on distributions of heights and lateral dimensions of "grains".

EXPERIMENTAL DETAILS

The $Si_{1-y}Ge_y$:H films were deposited by LF PECVD at substrate temperature T_s=300 °C and discharge frequency f=110 kHz from SiH_4 and GeH_4 feed gases diluted with hydrogen, argon or without dilution. Glass (Corning 1737) and crystalline silicon were used as substrates. Before deposition the wafers were cleaned by RCA cleaning (RCA I, at 80°C for 15 minutes, rinsing in DI water, RCA II at 80°C for 15 minutes, rinsing in DI water). The native oxide was removed in a HF:H_20 solution. Surface morphology measurements were conducted by an Atomic Force Microscope ("Quesant", model Q-scope 250). The AFM images in tapping regime for 2x2 μm^2 scan area were statistically analyzed. Average height roughness, <H>, heights distribution F(H), lateral correlation length, L_c, kurtosis, γ, were calculated from the AFM images. Additionally AFM images were analyzed with determining "grain" boundaries by the creation of threshold at 50% level and statistical analysis of the "grains" area F(S) and diameters F(D) distribution. Some of the films were isothermally annealed at T_a=400 °C for t=60 min in argon atmosphere.

RESULTS AND ANALYSIS

The surface morphology was studied as a function of Ge content in the films, Y, prepared with different dilutions. Fig. 1 shows the dependences of average heights <H> on Y. We can see that for H- and Ar dilution <H> increases by a factor of 2 when Y changes from 0.23 to 0.9. Meanwhile, for the films deposited without dilution, <H> increases more significantly from 3 to 35 nm, when Y changes from 0.3 to 0.8.

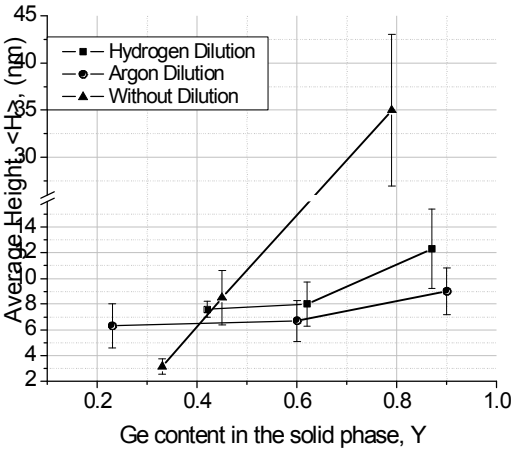

Figure 1. Average height as a function of Ge content, <H>(Y) for different gas dilutions. The films were deposited on silicon substrates.

Solid lines are a guide for the eye

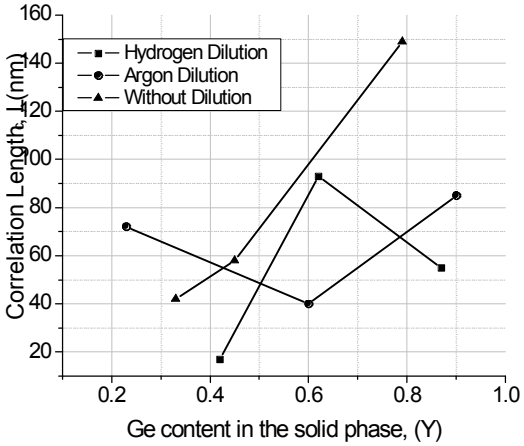

Figure 2. Correlation length as a function of Ge content, L_c(Y) for different gas dilutions. The films were deposited on silicon substrates. The error is 2 nm. Solid lines are a guide for the eye.

The lateral correlation length, L_c also changes with Y, as shown in Fig.2. L_c increases continuously with Y in the films deposited without dilution. The behavior of other films, however, is more complex: the films deposited with H-dilution demonstrate a maximum Lc =90 nm at Y=0.62, while the films deposited with Ar dilution shows a minimum Lc=40 in the same Y range.

Comparing the curves in Fig.1 and Fig. 2, one can see that some correlation between <H>(Y) and Lc (Y) is revealed only in the films deposited without dilution. No correlative trends are found for the films deposited with either H- or Ar dilution.

The "Sharpness" of height distribution is characterized by the parameter called kurtosis γ [18]. Its dependence on Ge content, Y, is shown in Fig. 3 for the films deposited with different dilutions. If $\gamma>3$, the width is narrower and if $\gamma<3$, the width is wider than that for corresponding Gaussian distribution. As can be seen in Fig. 3, narrow distributions are observed in two cases: in the films deposited with Ar dilution at Y=0.23 (γ= 5.3) and without dilution at Y=0.45 (γ= 4.3). In addition to L_c, we studied distribution of grain areas (diameters) by means of AFM image processing. Fig. 4 a) shows an example of an AFM image after creating grain "boundaries" at 50% threshold. The area distribution of grains F(S) can be calculated and, assuming circular shape for the grains, it is possible to get "diameter" distribution of grains, as shown in Fig. 4 b). The values of correlation length are observed to be close to the values of the diameters (e.g. see Table.1), but not for all the films studied. The reason for this discrepancy is not clear at present.

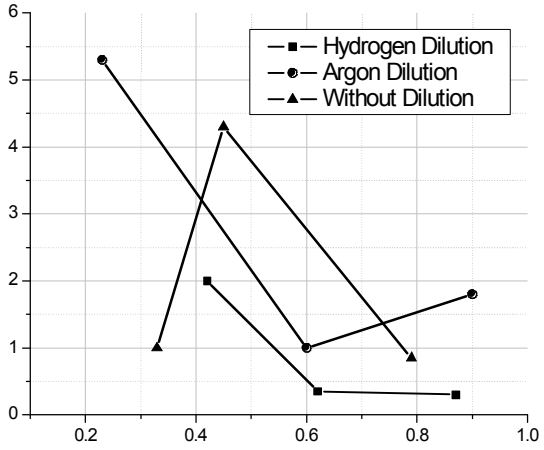

Figure 3. Kurtosis as a function of Ge content, Y, for different gas dilutions. The films were deposited on silicon substrates. Solid lines are guides for the eye. The error estimated is 0.25 (error determined from the calculation of the kurtosis in different images of the same scan size)

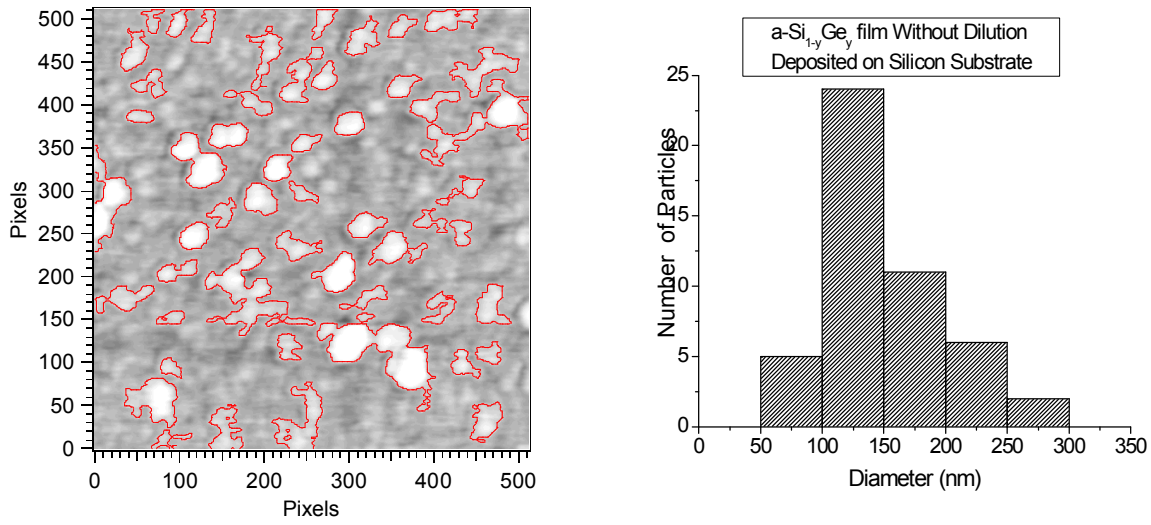

Figure 4. a) AFM image of the grains (1pixel =3.9 nm) and **b)** grain diameter distribution.

The changes in surface morphology observed after annealing, are indicated by the data in Table. 1. Annealing resulted in significant changes that depended on both dilution of feed gases and type of substrate. The latter is an important factor that can reverse the observed trends. Thus, on Si substrates, films prepared with H-dilution <H> reduces from 12.3 to 2.7 nm, while for the same films deposited on glass <H> increases from 6.4 to 15.6. In the films deposited on glass substrates, annealing causes <H> , L_c and <D> to increase for all dilutions. The films deposited on Si substrates demonstrate different trends depending on dilution. It is interesting to note that annealing results in significant sharpening of height distribution in the films deposited with H-dilution on Si substrate.

Table.1. Parameters for SiGe films deposited on silicon and glass substrates before and after annealing

Sample state	Average Height <H> ± R_a (nm)			Correlation Length Lc (nm)			Mean Diameter <D> (nm)			Kurtosis (γ)		
	Dilution			Dilution			Dilution			Dilution		
	H	Ar	No	H	Ar	No	H	Ar	No	H	Ar	No
	X = 0.5	X = 0.1	X = 0.2	X= 0.5	X= 0.1	X= 0.2	X= 0.5	X= 0.1	X= 0.2	X= 0.5	X= 0.1	X= 0.2
	Y = 0.87	Y = 0.23	Y = 0.45	Y= 0.87	Y= 0.23	Y= 0.45	Y= 0.87	Y= 0.23	Y= 0.45	Y= 0.87	Y= 0.23	Y= 0.45
As grown (on Si)	12.3 ± 3.1	6.3 ± 1.7	8.5 ± 2.1	55	72	58	95	107	131	0.3	5.3	4.3
As grown (on Glass)	6.4 ± 1.2	8.2 ± 2	16 ± 2.3	35	50	63	50	66	65	3.4	3.3	5.7
Annealed (on Si)	2.7 ± 0.6	40 ± 7.7	5.9 ± 1.6	60	199	62	160	657	103	65	0.5	4.7
Annealed (on Glass)	15.6 ± 2	70 ± 11	21 ± 5	110	145	150	1026	1042	998	1.2	0.2	0.3

CONCLUSIONS

We observed significant effects of feed gas dilution on morphology of Si-Ge films in the range of Y from 0.23 to 0.9. 1) <H> increases with Y in all cases: by a factor of 2 for both H- and Ar dilutions, reaching <H> 9-12 nm, and by a factor of 10 in the films deposited without dilution, reaching <H>=35 nm; 2) The correlation length continuously grows from $L_{c=}$42 nm to L_c=150 nm in the films deposited without dilution. The films prepared with H- and Ar- dilutions demonstrated more complex behavior: the former had a maximum L_c=95 nm and the latter a minimum L_c=40 nm at Y≈0.6; 3) The distribution of heights characterized by γ depended on dilution: narrow distributions with γ>3 were observed in the films deposited with Ar dilution (Y=0.23, γ=5.30) and without dilution (Y=0.45, γ= 4.3), while at higher Ge concentrations (Y>0.6) all the films demonstrated wide distributions with γ<3; 4) Isothermal annealing resulted in: a) an increase of <H> and L_c in the films deposited with H- and Ar- dilutions, while in the films prepared without dilution, the behavior was more complex: <H> increased on Si substrates but decreased on glass substrates. Also, L_c did not change on Si substrates but increased on glass substrate; 5) The width of the height distribution changed after annealing and significant narrowing of the distribution was observed in the films deposited with H-dilution or without dilution.

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